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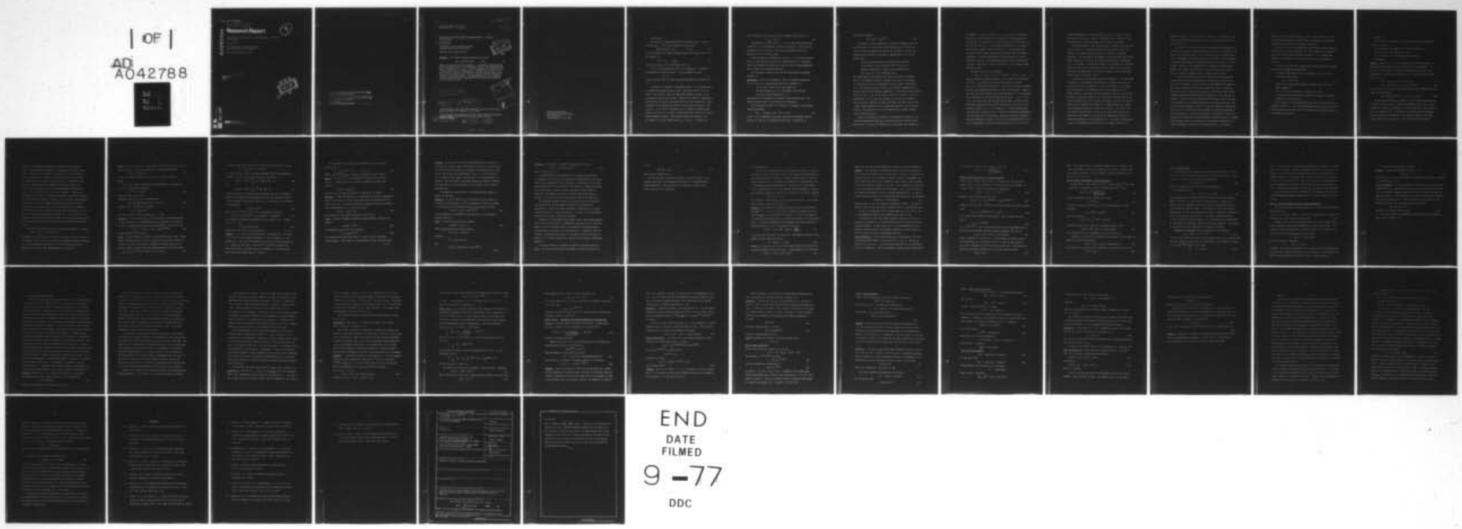

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Research Report

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THE CHOICE OF SMOOTHING NORM IN REGULARIZATION -- A KEY TO EFFECTIVENESS

Jane Cullum†

IBM Thomas J. Watson Research Center
Yorktown Heights, New York 10598

Typed by Lynne Bryant on MCST

IBM Research Division
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ABSTRACT: We consider ill-posed problems of the form

$$g(t) = \int_0^1 K(t,s)f(s)ds \qquad 0 \le t \le 1, \tag{1}$$

where g is given and we must compute f. The Tikhonov regularization procedure replaces (1) by a one-parameter family of minimization problems -- Minimize $(||Kf - g||^2 + \alpha\Omega(f))$ -- where Ω is a smoothing norm chosen by the user. We demonstrate by example that the choice of Ω is not simply a matter of convenience. We then show how this choice affects the convergence rate, and the condition of the problems generated by the regularization. An appropriate choice for Ω depends upon the character of the compactness of K and upon the smoothness of the desired solution.

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Copies may be requested from:
IBM Thomas J. Watson Research Center
Post Office Box 218
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1. Introduction

We consider ill-posed problems of the following type. Given a function $g(t)$, $0 \le t \le 1$, find a function $f(t)$ such that

$$\int_0^1 K(t,s)f(s)ds = g(t), \qquad 0 \le t \le 1. \tag{1}$$

In (1) we assume K is square-integrable and its null space, $N(K) = \{0\}$. For example, if

$$K(t,s) = \left.\begin{matrix} 1 & t>s \\ 0 & t<s \end{matrix}\right\}, \tag{2}$$

then the solution of (1) is the derivative of g.

From (1) using quadrature rules, we can generate -- in general rectangular but typically square -- linear algebraic systems

$$Ax = b, \tag{3}$$

where A has full rank and whose solutions approximate the solution of (1).

A problem is ill-posed in the Hadamard sense, if its solution does not depend continuously upon the data. Equations of type 1 are ill-posed. Note, however, that the associated algebraic systems (3) are well-posed, since A has full rank. However, for numerical computations problems must not only be well-posed, but also well-conditioned. Small variations in the problem data must not yield large variations in the solution. If we obtain the problem in (3) by applying standard quadrature rules to (1), it is easy to demonstrate that we obtain ill-conditioned algebraic systems. This happens because the operator in (1) is compact; i.e., its singular values $\sigma_n \downarrow 0$ as $n \uparrow \infty$. Recall that

each such operator has a singular value decomposition Smithies [1],

$$K = \sum_{n=1}^{\infty} \sigma_n v_n u_n^T . \tag{4}$$

The functions u_n and v_n, n=1, 2,... in (4) are eigenvector systems respectively, for the symmetric operators K*K and KK*. The σ_n^2 are the eigenvalues of K*K and the σ_n are called the singular values of K. Equality in (4) is in the L_2 sense.

Since the matrices A approximate K and $\sigma_n \downarrow 0$, the singular values of A will also converge to zero as the approximation to K is refined. Thus, A will become ill-conditioned. We note that for crude approximations, A may be fairly well-conditioned.

Our discussion focuses on the Tikhonov regularization procedure, Tikhonov [2].

<u>Definition 1</u>. We say a one-parameter family of problems, denoted by $P(\alpha)$ for $0 \le \alpha \le 1$, is a regularizing family for a problem P if

(a) For $0 \le \alpha \le 1$, each $P(\alpha)$ is well posed; and

(b) The solution f_α of $P(\alpha)$ converges to the solution f_0 of the original problem as $\alpha \downarrow 0$.

Convergence of the solutions is measured in some relevant norm. For numerical work we want at least pointwise convergence.

For an equation of type (1), Tikhonov [2] introduces the following regularizing family

$$P(\alpha) : \quad \text{Minimize} \quad ||Kf - g||^2 + \alpha\Omega(f). \tag{5}$$

In (5), $||\cdot||$ is typically an L_2-norm, measuring the residual error in solving (1), and $\Omega(f)$ is a smoothing norm which, in practice, is

typically set equal to

$$\Omega(f) = \int_0^1 f^2 + \int_0^1 (f^{(1)})^2. \tag{6}$$

The success of this procedure rests upon the assumption that the desired solution is smooth (has several derivatives), and that any errors in the data supplied are random and not smooth. We want the regularization procedure to generate an approximation to our given problem that

(a) is better conditioned, (b) mollifies the effects of any random noise in our data, and (c) gives us a physically meaningful solution that approximates the true solution in some reasonable sense.

We cannot achieve this objective by simply minimizing the residual error. The residual provides no measure of the lack of smoothness of a function f since the compactness of K may smooth oscillations in f. The residual controls only the low frequency components of f. Control over the high frequency components is exercised by the smoothing norm Ω in (5). $\Omega(f)$ will be small, only if f is smooth. Thus, the minimization in (5) forces the solutions f_α of the P_α to be smooth. Once we restrict ourselves to smooth functions, any such function with a small enough residual will be a good approximation to the true solution f_0. The selection of α in (5) determines the tradeoff between these 2 forms of control.

Much of the existing literature on regularization focuses on constructing regularizing families and proving that the required convergence occurs. In fact the implication in some papers (see Chechkin [3]

for example) is that the choice of Ω is a matter of convenience, and does not critically affect the behavior of the approximations. For kernels with singularities, there are results, such as Baglai [4], that tie the choice of Ω to the type of singularity in the kernel. We will argue, however, that the choice of Ω is important even for smooth kernels because numerical work demands more than simple convergence. The major application of regularization is to problems where the data is determined experimentally and contains noise or errors. When there is noise in the data, α in (5) cannot be made arbitrarily small.

We have, for any $\alpha \geq 0$ the inequality

$$||f(\alpha,\varepsilon) - f_0|| \leq || f(\alpha,\varepsilon) - f(\alpha,0)|| + ||f(\alpha,0) - f_0|| \quad (7)$$

where f_0 denotes the desired solution, $f(\alpha,0)$ denotes the solution of (5) with $g = g_0$, and $f(\alpha,\varepsilon)$ denotes the solution of (5) with $g = g_0 + \varepsilon$ for some error function ε. We note that we use ε to denote both an error function and the norm of this error function. Clearly, the size of the first term on the right-hand side of (7) is controlled by the condition of $P(\alpha)$ and the size of the error ε. If $\varepsilon \neq 0$, as $\alpha \downarrow 0$, this first term will get arbitrarily large. The size of the second term depends upon the rate of convergence of the $P(\alpha)$ to the original problem P, as $\alpha \downarrow 0$. Inequality (7) clearly demonstrates that there are 2 forces at work. To obtain a reasonable approximation, each $P(\alpha)$ must be well-conditioned, and we must achieve a reasonable rate of convergence. Clearly, if the rate of convergence of $P(\alpha)$ to P is not fast enough so that the noiseless solution $f(\alpha,0)$ of $P(\alpha)$ is

a good approximation to the true solution f_0 for $\alpha \neq 0$ and of a size determined by the noise ε, then it is unlikely that we will get a good approximation to our solution when there is error in the data.

We will demonstrate, for certain classes of operators and solutions, that the choice of Ω affects both the condition and the rate of convergence. Its effect upon the condition is, however, of primary importance. The condition of the members of the associated regularizing family improves as the order--the highest order derivative appearing in Ω--is increased. Increasing the order of Ω, generally has a negative effect upon the rate of convergence, but this effect is mollified and limited by the smoothness of the desired solution. This is explained in more detail in sections 3 and 4.

In section 2 we extend some results of Franklin [5]. He considered 3 problems: (a) the analytic continuation of a harmonic function that is known on a circle of radius $R < 1$ to the unit disk; (b) the backward heat equation in 1 dimension; and (c) the differentiation of a smooth function. He showed that the regularizing families obtained for the first 2 problems by using Ω_1 in (5) are poor approximations to the original problem when there is noise in the data. However, the corresponding family obtained for problem (c), differentiation, has reasonable convergence properties. He did not elaborate. In section 4 we will explain these results in terms of the small sensitivity of the condition of the members of the associated regularizing families to simple order changes in the smoothing norm Ω. This lack of sensitivity is due to the exponential decay rate of the singular values of the

associated operator. First, however, in section 2, we introduce norms that yield regularizing families that are 'good' approximations to problems (a) and (b).

In section 3, we consider in detail the problem of differentiating a function and derive relationships between the rate of convergence, the order of the smoothing norm Ω, and the smoothness of the desired solution. Furthermore, we demonstrate that the condition of the associated regularizing approximations generated improves as the order of Ω is increased, whereas the corresponding rate of convergence deteriorates. However, the overall error improves. The results derived in section 3 apply to a family of operators that includes differentiation.

In section 4 we extend the results obtained for differentiation to more general convolution equations. The results in section 4 are split into 5 theorems. The first theorem yields majorant estimates on the rate of convergence of Tikhonov regularizing families of order p for a large class of convolution operators. The second theorem yields minorant estimates on these rates for a subclass of the operators considered. Together these two theorems yield the exact order of the rate of convergence of the regularizing families for these subclasses. The third and fourth theorem in section 4, again for subclasses, relate the order of Ω to the condition of the approximating problems generated by the regularization. As for differentiation, increasing the order of Ω improves the condition of the corresponding regularizing family. Together these theorems yield, for a subclass of the operators considered, an overall estimate of the error in the approximations. We conclude

section 4 with a theorem that tells us that if our operator K is symmetric and positive definite, then there is a simplified regularizing family which we can use that is better conditioned.

Sections 3 and 4 use arguments which use Fourier transform analysis, similar to those given in Aref'eva [6]. We will discuss this paper as well as the earlier papers Arsenin and Ivanov [7], [8], Arsenin and Savelova [9], Goncharskii, Leonov, and Yagola [10] in more detail in section 4.

In section 5 we make some remarks about several ways that a regularization can be implemented numerically:

(a) Direct discretization of the functionals in (5) or of the associated Euler equation

$$(K^*K + \alpha B)f = K^*g \tag{8}$$

where B is the differential operator obtained from Ω by variational arguments.

(b) Use of Fourier transforms on equation (8), and

(c) Inversion of the differential operator B yielding an integral equation of the second kind.

The discussion is not chronological since some of the Russian work predates Franklin [5]. The results described give us heuristics for convolution equations that can be used in estimating the appropriateness of a proposed regularization.

2. Franklin [5]

In this section we examine the 2 classical ill-posed problems considered by Franklin [5]:

(a) The analytic continuation of a harmonic function in the unit circle (see equation (17)) and

(b) The solution of the backwards heat equation in 1-dimension.

Theorem 1. Franklin [5]. For the regularizing families obtained for problems (a) and (b) above, using the norm in (6) and assuming $d_1\varepsilon^2 \le \alpha \le d_2\varepsilon^2$, one obtains the following estimates of the error in the approximation of the desired solution f_0 by the solution $f(\alpha,\varepsilon)$ of $P(\alpha)$ with $g_\varepsilon = g_0 + \varepsilon$,

$$\text{(a)} \qquad ||f(\alpha,\varepsilon) - f_0|| \le [C_1/(-\ell n\alpha)] \tag{9}$$

$$\text{(b)} \qquad ||f(\alpha,\varepsilon) - f_0|| \le C_2\,[T/(-\ell n\alpha)]^{p/2}. \tag{10}$$

In (10) [0,T] is the interval of interest for the heat equation, and this result was obtained with

$$\Omega_p(f) = \sum_{j=0}^{p} m_j ||f^{(j)}||_2^2 \qquad p = 1,2,\ldots, m_j \ge 0 \tag{11}$$

We note that the setting in Franklin [5] is different from what we will use in later sections. Franklin considered varying α and ε simultaneously. He asked the question: If $||Ku|| \le \varepsilon$ and $\Omega(u) \le 1$, then how does the $||u||$ behave as $\varepsilon \downarrow 0$? He called this the modulus of regularization. In his arguments, he proved that if we consider functions u such that $\Omega(u) \le Q$, then using 2 choices for ε and Q he can bound the ordinary

modulus of convergence by multiples of the modulus of regularization. Thus, estimating the modulus of regularization yields a corresponding estimate on the modulus of convergence as ε and α decrease to zero. The estimates in (9) and (10) were obtained using the modulus of regularization and assuming that $d_1\varepsilon^2 \le \alpha \le d_2\varepsilon^2$. The Franklin arguments [5] used Fourier series expansions of the solutions of the (a) analytic continuation and (b) the backwards heat equation problems. In this section we will use similar arguments to derive error estimates for other norms. The class of problems considered in section 4 will include these 2 problems. However, we also consider them separately here because Franklin's arguments [5] explicitly relate the control exercised by the residual term in (5) to the low frequency components of the solution and the control exercised by the smoothing norm Ω in (5) to the high frequency components of the solution. In section 4 we will demonstrate using Fourier transform analysis that the high frequency norm control is the mollifier of the condition of the regularizing approximations.

If we know for problem (a) that for the desired solution the quantity

$$\Omega_\infty^c\ (f) = \sum_{j=0}^{\infty} ||f^{(j)}||^2 c^{2j}/(2j)! \tag{12}$$

exists and is finite for some $c>0$, where the L_2-norm is over the interval of interest, then we can use Ω_∞^c to define a regularizing family for problem (a). We will demonstrate that for $c \ge -2\ell nR$, the regularizing family generated by Ω_∞^c yields 'good' approximations to problem (a).

Lemma 1. Let f be C^∞ on $(-\infty,\infty)$ and assume $f^{(j)}(t)\to 0$ as $|t|\to\infty$ for $j=0,1,2...$ Assume also that the Fourier transform of f exists and satisfies

$$|\hat{f}(\omega)| \le M \exp(-\mu|\omega|) \tag{13}$$

for all $|\omega|>S$ and for some $M>0$. Then, if $2\mu>c$, $\Omega^c_\infty(f)$ is finite.

Proof.

By (13) the Fourier transform of each derivative of f exists and is in L_1. By Parseval's equality,

$$||f^{(j)}||^2 \le ||\omega^j \hat{f}||^2 \tag{14}$$

where the ω-norm is on $(-\infty,\infty)$.

Therefore, each term in (12) is majorized by

$$\left(\bar{M}/(2j)!\right) \int_0^\infty (c\omega)^{2j} \exp(-2\mu|\omega|) \le \bar{M}\,(c/2\mu)^{2j} \tag{15}$$

Combining (15), (14) and (12) we obtain

$$\Omega^c_\infty(f) \le \bar{M} \sum_{j=0}^{\infty} (c/2\mu)^{2j}.$$

But, this series is finite, whenever $2\mu>c$. Q.E.D.

Theorem 2. If for the solution f_0 of the analytic continuation problem $\Omega^c_\infty(f_0)<\infty$, then for the regularizing family P_α defined in (5) using Ω^c_∞ in (12), we obtain the following majorant estimate of the error as $\alpha\downarrow 0$,

$$||h_\alpha||^2 \equiv ||f(\alpha,\varepsilon) - f_0||^2 \le Q^*\alpha^{c/(c-2\ell nR)} \tag{16}$$

We have assumed that $d_1\varepsilon^2 \le \alpha \le d_2\varepsilon^2$.

Proof. We repeat Franklin's analysis, using instead the Ω^c_∞- norm. We are given a harmonic function $u(r,\theta)$ in the unit disk with known values for some $R<1$, $g_0= u(R,\theta)$, and asked to determine its values $f_0=u(1,\theta)$ on the unit circle. We must solve the integral equation of the first kind,

$$g_0 = 1/2\pi \int_0^{2\pi} [1-R^2/1-R\cos(\theta-\theta_1)+R^2]\; f_0(\theta_1)d\theta_1 \;. \tag{17}$$

We know the solution is periodic so we write the error $h_\alpha = f(\alpha,\varepsilon) - f_0$ as

$$h_\alpha(\theta) = \sum_{n=0}^{\infty} (A_n \cos n\theta + B_n \sin n\theta) \ .$$

If $||Kh_\alpha||^2 \le \alpha\bar{Q}$ and $\Omega_\infty^c(f_0) < Q$ we obtain, assuming that the interchanges of summation, integration, and differentiation are correct,

$$\Omega_\infty^c(h_\alpha) = 2\pi A_0^2 + \pi \sum_{n=1}^{\infty} \cosh(cn)(A_n^2 + B_n^2) \le 2Q \tag{18}$$

and

$$||Kh_\alpha||^2 = 2\pi A_0^2 + \pi \sum_{n=1}^{\infty} R^{2n}(A_n^2 + B_n^2) \le \alpha\bar{Q} \ . \tag{19}$$

Following Franklin, we balance the contribution from the low frequency terms in (19) against the contribution from the high frequency terms in (18) by choosing an appropriate value for n. Let $N=N(\alpha)$ be the solution of the equation

$$\alpha \cosh cN = 2R^{2N} \ . \tag{20}$$

Since for $n \le N$, $R^{2n} \ge R^{2N}$; and for $n>N$, $\cosh cn > \cosh cN$, we obtain

$$||h_\alpha||^2 \le ||Kh_\alpha||^2 R^{-2N} + \Omega(h_\alpha)(\cosh cN)^{-1} \le 2\bar{Q}(\cosh cN)^{-1}. \tag{21}$$

Now consider the asymptotic behavior of N as a function of α. Clearly, as $\alpha \downarrow 0$, $N \uparrow \infty$, and

$$N \sim \left(1/(c - 2\ln R)\right) \ln(4/\alpha) \ . \tag{22}$$

Substituting (22) into (21) we obtain (16). Q. E. D.

<u>Comments</u>. If $c = -2\ln R$, then the exponent in (16) equals 1/2. For fixed R, as we let $c \uparrow \infty$ this exponent approaches 1. As we decrease c, it decreases to 0. Note that the eigenvalues of K*K decay like $\exp(2n\ln R)$ as $n \uparrow \infty$. Choosing a norm with a growth rate that matches or exceeds this decay rate yields a reasonable rate of convergence. To use Ω_∞^c we must know that for the desired solution $\Omega_\infty^c(f_0) < \infty$.

We can achieve a better rate of convergence if we use an even stronger norm.

$$\bar{\Omega}_{\infty}^{c} \equiv \sum_{j=0}^{\infty} c^{j}||f^{(j)}||^{2}/j! \qquad \text{for } c>0 \tag{23}$$

Then we have the following; the proof is similar to that of Lemma 1.

Lemma 2. Let $f \in C^{\infty}$ on $(-\infty,\infty)$ and assume $f^{(j)}(t) \to 0$ as $|t| \to \infty$ for all $j=0,1,2...$ Assume also that the Fourier transform of f exists and satisfies,

$$|\hat{f}(\omega)| \leq M \exp(-\mu\omega^{2}) \tag{24}$$

for all $|\omega|>S$, for some $M>0$ and $\mu>c/2$. Then $\bar{\Omega}_{\infty}^{c}$ (f) is finite.

Theorem 3. *If for the solution* f_0 *of the problem of analytic continuation* $\bar{\Omega}_{\infty}^{c}(f_0)<\infty$, *for some* $c>0$, *then for the regularizing family defined in (5) using* $\bar{\Omega}_{\infty}^{c}$ *in (23), we obtain the following majorant estimate of the error in the approximation as* $\alpha,\varepsilon \downarrow 0$ *with* $d_1\varepsilon^2 \leq \alpha \leq d_2\varepsilon^2$,

$$||f(\alpha,\varepsilon) - f_0||^{2} \leq Q^{*}\alpha \quad . \tag{25}$$

This estimate is also valid for general α and R near 1.

Proof. The proof proceeds as before with small changes. Equation (20) becomes

$$\alpha \exp(cN^{2}) = 2R^{2N} \quad . \tag{26}$$

The asymptotic solution of this satisfies

$$N \sim (-\ell n(\alpha/2)/c)^{1/2} \quad . \tag{27}$$

for a given R and sufficiently small α, or for a given α and sufficiently large R. Then using (27) and the analog of (21), we obtain (25).

Q.E.D.

<u>Comments</u>. We note that to use Ω_∞^c or $\bar{\Omega}_\infty^c$ numerically we would have to use Fourier transforms, and we would have to know that our desired solution had sufficient smoothness to guarantee the existence of Ω_∞^c or $\bar{\Omega}_\infty^c$. We note that as $R\downarrow 0$, the eigenvalues R^n, $n=1,2,\ldots$ of the operator K in (17) decrease more rapidly, and the error in the approximation increases. Thus, by picking a norm whose growth rate matches or exceeds the decay rate of the given operator, we can achieve 'good' orders of approximation.

If we apply the same analysis to the backwards heat equation we obtain the following.

<u>Theorem 4</u>. If for the solution f_0 of the backwards heat equation in 1-dimension we have $\bar{\Omega}_\infty^c(f_0)<\infty$, then the regularizing family P_α defined in (5) using $\bar{\Omega}_\infty^c$ in (23) satisfies the following majorant estimate

$$||f(\alpha,\varepsilon) - f_0||^2 \le Q^*\alpha^{c/(c+2T)} \tag{28}$$

The heat equation is considered on the interval $(0,T)$, and again we assume $d_1\varepsilon^2\le\alpha\le d_2\varepsilon^2$.

<u>Proof</u>. In this case we obtain the equation

$$\alpha \exp(N^2(c + 2T)) = 2 \tag{29}$$

Taking logarithms of both sides we obtain,

$$N^2(c + 2T) = -\ell n(\alpha/2) .$$

Therefore,

$$N^2 = -\ell n(\alpha/2)/(c+2T)$$

and

$$||h_\alpha||^2 \le \bar{Q} \exp(-cN^2) \le Q^*\alpha^{c/(c+2T)}$$

Q.E.D.

Theorem 5. If we use Ω_∞^c, we obtain an estimate of the form

$$||h_\alpha||^2 \le Q^* \exp(-\bar{c}(-\ell n\alpha)^{1/2}) \tag{30}$$

where $\bar{c}$ involves c and T.

The difference in the convergence of the regularizing families for problems (a) and (b) can be explained by the difference in the decay rates of the eigenvalues of the 2 operators. For problem (a) the eigenvalues decay like R^n; for problem (b) like $\exp(-n^2T)$. Thus, the norm Ω_∞^c with a growth rate of exp(cn) cannot counteract the rapid decay of $\exp(-n^2T)$. For problem (b) we must go to $\bar{\Omega}_\infty^c$, whose growth rate is $\exp(cn^2)$, to achieve an overall approximation that is some power of α.

The preceding analysis points out the need to have an estimate of the decay rate of the given operator K as an aid in choosing an appropriate Ω. We are of course constrained in what order Ω we can use by the smoothness of the desired solution. In order for the convergence arguments to be valid, $\Omega(f_0)$ must be defined.

Arguments of the preceding type assumed α and ε varied simultaneously and in fact that $d_1\varepsilon^2 \le \alpha \le d_2\varepsilon^2$. Consequently, the effect of Ω on the individual rates of convergence and on the condition of the approximating problems cannot be obtained from such arguments. In sections 3 and 4 we attempt to estimate directly rates of convergence, and the condition of members of the Tikhonov regularizing families of more general convolution operators.

In the next section, we examine the problem of differentiation in detail. We will be using Fourier transforms so instead of equation (1)

we use

$$\int_{\infty}^{t} f(s)ds = g(t) \qquad -\infty<t<\infty \qquad (31)$$

where we have assumed $g(-\infty)=0$.

We will show that increasing the order of Ω makes the rate of convergence deteriorate, but improves the condition of the approximating problems generated. The net effect is to improve the overall error $||f(\alpha,\varepsilon)-f_0||$ if $\alpha<C\varepsilon^2$ for some C.

3. Differentiation.

Now let us use differentiation to understand the effect on the rate of convergence and on the conditioning of the regularizing approximations for various choices of the norm Ω. We want to demonstrate the interplay between the choice of Ω, the rate of convergence, the conditioning, and the smoothness of the desired solution. We will work on the interval $(-\infty,\infty)$ using equation (31), and use Fourier transform analysis. In fact, the following theorems are valid for any operator K with Fourier transform

$$|\hat{K}(\omega)| = D\omega^{-r},\ r>0\ . \tag{32}$$

This includes, in particular, all the derivative operators. We use arguments similar to those in Aref'eva [6].

<u>Theorem 6</u>. We assume that the desired solution f_0 has $m\geq 1$ derivatives, that each $f^{(j)} \in L_1(-\infty,\infty)$ $0\leq j\leq m$, and its Fourier transform $\hat{f}$ satisfies $|\omega^{j+1}\hat{f}|<R_{j+1}$ for all ω and $|\hat{f}|>D_1\omega^{-m-1}$ for large ω. Then for any equation (1) whose kernel K satisfies (32), we have the following. For sufficiently small α, the rate of convergence of the Tikhonov regularizing families obtained using Ω_p in (11), for $m\leq 2p+2r-1/2$ varies as

$$||f(\alpha,0) - f_0|| \leq Q\alpha^a \quad \text{where } a = \frac{2m+1}{4p+4r}\ . \tag{33}$$

For $m>2p+2r-1/2$ this rate is at least $O(\alpha)$. The dynamic condition of the members of these families varies as

$$\alpha^b\ , \text{ where } b = -r/(p+r) \tag{34}$$

Moreover, for any $m\geq 1$, $p\geq 0$, and $r>0$, an overall estimate of the error in using the solution of $P(\alpha)$ with $g_\varepsilon=g_0+\varepsilon$ to approximate f_0 is of the form,

$$||f(\alpha,\varepsilon) - f_0|| \leq C_1\alpha^q + \varepsilon C_2\alpha^b \tag{35}$$

where $b=-r/(p+r)$ and $q=(2m+1)/(4p+4r)$ if $m\le 2p+2r-1/2$, and $q\ge 1$ otherwise.

Comments. The smoothness of the solution helps the rate of convergence, but of course does nothing for the error term. Using (35), we see that increasing the order p of Ω adversely affects the rate of convergence, but has a significant effect on the condition, which typically would outweigh in (35) any negative influence on the rate. As we increase the decay rate r of K, the condition and the rate deteriorate. As $r\uparrow\infty$ the estimate of the condition approaches $1/\alpha$ and of the rate approaches $O(1)$. If we fix r and increase the order p, the convergence rate estimate in (33) approaches

$$\alpha^{e} \text{ where } e = (2m+1)/(4m+4r) \tag{36}$$

since $p\le m$; and in (34), the exponent b approaches $-r/(m+r)$. We show in Theorem 7 that in fact the optimal estimate in (35) is achieved when p=m.

By rate of convergence, we will always mean the size of the L_2-norm of the discrepancy caused by the regularization, $h_\alpha=f(\alpha,0)-f_0$.

By condition we mean the dynamic condition Makhoul [11] which is a measure of the difficulty of the deconvolution of the associated Fourier transform problem. In cases where the discrete approximation used is a symmetric Toeplitz matrix, the algebraic condition of these matrices is not worse than that given by the dynamic condition.

Proof of Theorem 6. First consider the rate of convergence of the associated regularizing family as a function of p, m, and r. Consider Ω_p given by (11) for p=1,2... We use Fourier transforms and the Euler equation (8) to compute f_α. Then the discrepancy caused by the regularization

$h_\alpha = f(\alpha,0)-f_0$, using Parseval's equality, satisfies

$$||h_\alpha||^2 = \alpha^2 \int_0^\infty \frac{\omega^{4p+4r}\hat{f}^2}{(\bar{c}+\alpha\omega^{2p+2r})^2\pi} \tag{37}$$

Part a: Rate of convergence - Majorant estimate

We split this integral into the sum of integrals over $(0,M)$ and (M,∞) where M will be chosen subsequently to optimize the error estimate. If we have $|\omega^j\hat{f}|^2 < R_j$, then we have for any M, and $0<j\leq m+1$

$$\int_M^\infty |\hat{h}_\alpha|^2 \leq R_j \int_M^\infty \omega^{-2j} = \bar{R}_j M^{-2j+1} \quad . \tag{38}$$

Moreover, for $0\leq j\leq J=\min(2p+2r+1/2,\ m+1)$

$$\int_0^M |\hat{h}_\alpha|^2 \leq R_j\alpha^2 \int_0^M \omega^{4p+4r-2j} = R_j^*\alpha^2 M^{4p+4r-2j+1} \quad . \tag{39}$$

Combining (38) and (39), we obtain the majorant estimate for any $j\leq J$ of the form,

$$||h_\alpha||^2 \leq E_1\alpha^2 M^{4p+4r-2j+1} + E_2 M^{1-2j} \quad . \tag{40}$$

If we choose M to minimize the expression in (40), we obtain for each such j,

$$M_j = C\alpha^{-1/(2p+2r)} \tag{41}$$

or $\alpha = \bar{C}M^{-(2p+2r)}$. Thus, the optimal choice of M is independent of $j\leq J$, and we obtain the optimal majorant estimate obtainable from (40) as

$$||h_\alpha||^2 \leq Q_j\alpha^a \quad \text{with } a = (2j-1)/(2p+2r) \tag{42}$$

where Q_j depends on j but not on α. In particular for a given r and p, if the smoothness of f satisfies $m\leq 2p+2r-1/2$, then the best order of α in (42) corresponds to $j=m+1$ for which we obtain (33). If $m>2p+2r-1/2$, then the best order is obtained with $j=2p+2r+1/2$ when we obtain

$$||h_\alpha||^2 \leq \bar{Q}\alpha^2 \quad . \tag{43}$$

Note. The constant terms in the various equations do not involve α and do not significantly affect the arguments so no attempts have been made to be precise with them. We note, moreover, that the estimates in (42) and (43) hold for all $\alpha>0$.

Part b: Rate of Convergence - Minorant Estimate

We must obtain a lower bound on $||h_\alpha||^2$. Since $|\hat{f}|>D_1\omega^{-m-1}$ for large ω and $|\hat{K}|=D\omega^{-r}$ everywhere, we have for sufficiently small α that

$$||h_\alpha||^2 \geq \bar{C} \int_M^\infty \frac{\alpha^2\omega^{4p+4r-2m-2}}{(1+\alpha\omega^{2p+2r})^2} \tag{44}$$

where M is defined in (41). But for $\omega>M$ we have

$$\alpha\omega^{2p+2r}>C>0 \ . \tag{45}$$

Therefore, we have with $Q=(C+1)/C$, on (M,∞) the denominator in (44) satisfies,

$$(1 + \alpha\omega^{2p+2r}) \leq Q\alpha\omega^{2p+2r} \quad . \tag{46}$$

From (46) we obtain

$$||h_\alpha||^2 \geq \bar{Q} \int_M^\infty \omega^{-2m-2} = Q^*M^{-2m-1} \quad .$$

Therefore, using (41) we obtain for sufficiently small α that

$$||h_\alpha||^2 \geq \bar{Q}\alpha^a \ \text{ with } \ a = (2m+1)/(2p+2r) \ . \tag{47}$$

The coefficient $\bar{Q}$ in (47) depends on p, m, and r but not α.

Combining (33) and (47) for $m\leq 2p+2r-1/2$, we obtain an exact order estimate of the rate of convergence

$$||h_\alpha||^2 \leq Q_1\alpha^a \ \text{ with } a = (2m+1)/(2p+2r) \quad . \tag{48}$$

For $m>2p+2r-1/2$, we get that the convergence is at least as fast as α^2

$$||h_\alpha||^2 \leq Q_2\alpha^2 \tag{49}$$

Part c. Conditioning

The condition of a minimization problem typically refers to the condition of the second derivative operator of the given functional. In our case this is the operator in the Euler equation (8)

$$\phi = K^*K + \alpha B \tag{50}$$

where B is generated from Ω using variational arguments.

For differentiation,

$$\phi(f) = \int_t^1 \int_0^s f + \alpha f - \alpha f^{(2)} \quad . \tag{51}$$

If we approximate this operator and f by discretizing, then we obtain a matrix. However, the type of matrix obtained Toeplitz, symmetric etc. depends upon the quadrature rule used for K*K and the approximation of the differential operator chosen. The algebraic condition may vary depending upon the particular approximation chosen. Therefore, we choose to look at this operator directly and to use Fourier transform analysis. We use the dynamic condition, Makhoul [11], the maximum and minimum values of the modulus of the Fourier transform of our given operator. This notion of conditioning is only applicable to convolution operators.

Therefore, we form the Fourier transform of ϕ, and consider

$$h(\omega) = |\hat{\phi}(\omega)| = \omega^{-2r} + \alpha\omega^{2p} \tag{52}$$

In (52) we have ignored the lower order derivative terms in Ω_p, because they have only secondary effects upon the conclusions. The minimum of h occurs at $\omega=(r/p\alpha)^{1/(2p+2r)}$ and is of the order

$$C\alpha^a, \quad a = r/(r+p) \quad . \tag{53}$$

(53) is a lower bound on the smallest eigenvalue of the operator ϕ. Observe that ϕ has no maximum. However, in numerical work, there is a limit on the sampling size, and the maximal singular value of any discretization of ϕ depends primarily on this sample size. To see this consider the following. We know, see e.g. Wilkinson [12], that for any matrix A that approximates K, all the eigenvalues of A satisfy $|\lambda_j(A)| \le ||A||$ for any consistent matrix norm. In particular the maximal row sum norm is a bound on the eigenvalues.

So we can conclude that as the order of Ω is increased, the condition of the approximating problems improve, and the critical order in α is given in (34).

Part d. Overall Estimate of Error in the Approximation

Now let us consider the overall error in (7). Using Fourier transforms we find that the

$$||f(\alpha,\varepsilon) - f(\alpha,0)||^2 = ||\hat{f}(\alpha,\varepsilon) - \hat{f}(\alpha,0)||^2 \le C_2\varepsilon\alpha^b \text{ with } b = -r/(2r+2p) \quad (54)$$

Combining (54), (48) and (52) we obtain (35). Q.E.D.

Theorem 5 tells us that for small decay rates r we can achieve fairly well-conditioned, approximating problems with a small order norm Ω. For computing the first derivative of a function we have r=1. Therefore, for $m \le 2p+3/2$ we have the convergence rate is of order

$$\alpha^a \quad \text{with } a = (2m+1)/(2p+2)$$

and the condition is bounded by

$$C\alpha^b \quad \text{with } b = -1/(p+1) .$$

Therefore, for a given m and $p > m/2-3/4$, we have that the rate becomes worse as we let $p \uparrow m$. At p=m the convergence rate is nearly 1. The condition improves significantly as $p \uparrow m$, its best value is achieved when p=m.

We have the following simple theorem.

Theorem 7. Under the hypotheses of Theorem 6, for

$$\alpha < (C_2\varepsilon/C_1)^2 \tag{55}$$

and $m \le 2p+2r-1/2$, the choice Ω_m yields the regularizing family that minimizes the overall error in (35).

Proof of Theorem 7. We can approximate the minimum of (35) by solving the equation $\alpha^b = \varepsilon c_2/c_1$ where $b=(m+1/2+r)/(2r+2p)$ for p since the first term in (35) is a monotone increasing function of p and the second a monotone decreasing function. If the solution lies in the interval $p \ge m$ then the minimum value corresponds to $p=m$. Taking logarithms of both sides of this equation and using (55) we get the solution p^* satisfies

$$2p^* + 2r > 2m + 2r + 1 .$$

Therefore, the optimal choice is $p=m$. Q.E.D.

In the next section we consider more general convolution operators, again on the interval $(-\infty,\infty)$.

4. General Convolution Equations.

In this section we extend the results obtained in the previous section for operators of the form $|\hat{K}(\omega)|=C\omega^{-r}$, $r>0$, to more general convolution equations. Arsenin and Ivanov [7], Arsenin and Savelova [9], Goncharski, Leonov and Yagola [10] and Aref'eva [6] have each derived estimates on the asymptotic rates of convergence (as $\alpha\downarrow 0$), and on the overall error bounds attainable when the data is inaccurate, for certain classes of convolution equations on the interval $(-\infty,\infty)$. Each paper used Fourier transform analysis. The families considered in Aref'eva [6] will be described. These include those considered in the other papers. The papers are listed chronologically. The Arsenin and Ivanov [7] and Arsenin and Savelova [9] papers obtained majorant estimates that relate the decay of the transform of the operator K, the order of the norm Ω, and the smoothness of the desired solution. They used complex variable theory to evaluate the error integrals. Goncharski, Leonov and Yagola [10] enlarged the class of kernels under consideration and used the L_2-norm of the Fourier transform of the error so they could work with real integrals. However, they did not consider general norms Ω or the effects of the smoothness of the desired solution. Aref'eva [6] considered the same class of kernels as in [10]. However, he answered a slightly different question. Generalizing the class of admissible regularizers, he obtained the following Theorem. For a precise statement see Aref'eva [6].

<u>Theorem 8</u>. Aref'eva [6]. For a given level of noise, σ, the optimal approximation f_σ to the desired solution of (1) is obtained with

$$\hat{B} = \sigma^2/|\hat{f}_0|^2 \tag{56}$$

where $\hat{B}$ is the transform of the operator B in (8).

Thus, in the presence of noise, the optimal choice of regularizer depends only on the decay rate of the Fourier transform of the desired solution. We note that the expression in (56) may or may not have a function analytic interpretation as the norm of some identifiable function space. All Tikhonov regularizers are, of course, defined initially in terms of such norms. Using (56), Aref'eva [6] derives estimates on the optimal error achieved in terms of σ. Since (56) is not a priori computable, Aref'eva then returns to Tikhonov regularizers and shows that order-wise, for certain classes of problems, he can achieve to the same order the error that he gets using the optimal regularizer in (56). For certain subclasses he obtains order exact estimates.

In this paper we consider only Tikhonov regularizers. When we make this restriction then the character of the compactness of the operator and the smoothness of the desired solution are both of primary importance. The character of the compactness of K determines whether or not the approximation obtained using a particular family of regularizers is sufficient to make sense computationally. As we saw in section 2 with exponentially decaying operators K, in order to obtain an approximation of the order α^a for some a>0, we had to use an exponentially increasing smoother Ω_∞^c. Obviously, the use of Ω_∞^c is limited by the smoothness of our desired solution. The convergence arguments are valid only when $\Omega(f_0)$ is defined.

Numerically, we have to worry about the condition of the approximating problems generated. As in section 3, we will use the dynamic condition.

The discussion has 3 parts. First for a large class of operators we obtain in Theorem 9 a majorant estimate of the rate of convergence of the approximating regularizing family when there is no noise. In Theorem 10 for a subclass of these operators we obtain a minorant estimate of this rate. Together Theorems 9 and 10 give us the order of the rate of convergence for this subclass. In Theorems 11 and 12 for a further subclass we estimate the dynamic condition of the approximating problems generated using Ω_p (Theorem 11) and using Ω_∞^c and $\bar{\Omega}_\infty^c$ (Theorem 12). Together these theorems give us an estimate on the overall behavior of the error in approximating our given solution f_0 by the solution of $P(\alpha)$ for $g=g_0+\varepsilon$.

Using these estimates we can argue that typically one would obtain the best error by maximizing the order of Ω. For a function f_0 with m derivatives this corresponds to taking p=m. We note, however, that in practice we often do not know m and we are likely to choose a low order Ω because it is easier to work with. In such a situation it is important to have some estimate of the decay rate of our operator. Since we are nominally working with symmetric, Toeplitz operators the associated Fourier transforms give us such an estimate. Using this estimated decay rate we can use the inequalities obtained to indicate whether the proposed regularization makes sense numerically.

The following are slight modifications of definitions in Aref'eva [6].

Definition 2. Aref'eva [6]. A kernel K is of type 1 if (a) Its transform, $|\hat{K}(\omega)|$ has a denumerable number of zeros on the real axis of ω. (b) There are no limit points for the zeros of $\hat{K}(\omega)$ with the exception of $\omega=+\infty$, and if

$N(M)$ is the number of zeros in $(0,M)$, then $N(M) \le CM^{\nu}$ for some $\nu \ge 0$, $C \ge 0$; (c) There exists a system of non-overlapping ε-neighborhoods of the zeros of $\hat{K}(\omega)$ on $\omega \ge 0$ such that $|\hat{K}(\omega)| \ge a_i |\omega - \omega_i|^s$ for $\omega \varepsilon [\omega_i - \varepsilon_i, \omega_i + \varepsilon_i]$ where the $\omega_i > 0$ are the finite, nonzero, zeros of $\hat{K}$ and $a_i \ge a > 0$, $s > 0$. (d) If $\hat{K}(0) \ne 0$, then there is an interval $[0, \varepsilon_0)$ in which $|\hat{K}(\omega)| > C$. (e) Outside these ε-neighborhoods, $|\hat{K}(\omega)| \ge D\, \omega^{-r}$, $r > 0$, $D > 0$.

We note that $\hat{K}$ can have infinitely many zeros satisfying (c) only if $\varepsilon_i \to 0$ as $i \to \infty$.

Definition 3. Aref'eva [6]. A kernel is of type 2 if for large ω $|\hat{K}(\omega)| \ge C \exp(-A\omega)$ for some $A > 0$, $C > 0$.

Within type 1 Aref'eva [6] determines a subclass for which he also derives a lower bound estimate of the same order. Aref'eva [6] also classifies solutions f_0 in terms of the behavior of their Fourier transforms. He further subdivides type 1 into $0 \le s < 1/2$, integrable singularities and $s > 1/2$, nonintegrable singularities. We consider only $s < 1/4$. We use Aref'eva type arguments to derive our estimates in Theorems 9 and 10. We note that the arguments in section 3 also mimic Aref'eva [6] arguments.

Theorem 9. Consider the norms Ω_p $p \ge 1$ and equation (1). Let the solution f_0 of (1) have $m \ge 1$ derivatives with each $f^{(j)} \varepsilon L_1(-\infty, \infty)$, $0 \le j \le m$ and $|\omega^{j+1} \hat{f}(\omega)| \le R_{j+1}$ for all ω. (a) Let K be of type 1 with $0 \le s < 1/4$ and $\nu \le 4s$. Then the discrepancy $h_\alpha \equiv f(\alpha, 0) - f_0$ satisfies the following.

For $p \ge m/2 - r + 1/4$,

$$||h_\alpha||^2 \le C_1 \alpha^b \quad \text{with } b = (2m+1)/(2p+2r) \tag{57}$$

and for $p < m/2 - r + 1/4$, $||h_\alpha||^2 \le C_2 \alpha^2$.

(b) Let K be of type 2 with $|\hat{K}| \geq D\exp(-a\omega)$ for some $a>0$ and for all ω. Then

$$||h_\alpha||^2 \leq C_3(-\ell n\alpha)^{-(2m+1)} \quad . \tag{58}$$

In (57) p is the order of Ω, r is the decay rate of $|\hat{K}|$, and s and ν are as specified in definition 2.

Proof - Part a. (The argument parallels that in Theorem 2 of Aref'eva [6].) The proof is analogous to that given for Theorem 5, using expression (37) for $||h_\alpha||^2$ except that it is now necessary to split the integral over $(0,M)$ into integrals over neighborhoods of the zeros of $\hat{K}$, and integrals over the complements of these neighborhoods. For each neighborhood $N_i=(\omega_i-\varepsilon_i,\omega_i+\varepsilon_i)$ of a zero ω_i of $|\hat{K}|$ we have

$$\int_{N_i} |\hat{h}_\alpha|^2 \leq \alpha^2 \int_{N_i} \frac{\omega^{4p}|\hat{f}|^2}{|\omega-\omega_i|^{4s}} \leq \bar{C}\alpha^2\varepsilon_i^{1-4s}$$

There are at most M^ν such intervals in $(0,M)$ and clearly each $\varepsilon_i<M$, so we obtain

$$\sum_i \int_{N_i} |\hat{h}_\alpha|^2 \leq \bar{C}\alpha^2 M^{1-4s+\nu}$$

Now consider the integrals over the complements $\bar{N}_i$ of the N_i. On the complements $|\hat{K}|>D\omega^{-r}$

$$\sum_i \int_{\bar{N}_i} |\hat{h}_\alpha|^2 \leq \bar{D}\alpha^2 \int_0^M \omega^{4p+4r}\ |\hat{f}|^2 \leq \alpha^2 D_j M^{4p+4r-2j+1}$$

for any $j\leq J=\min(m+1,\ 2p+2r+1/2)$.

The integral from (M,∞), as in Theorem 5, satisfies (44). Therefore,

$$||h_\alpha||^2 \leq \alpha^2\bar{C}M^\mu + D_j M^{1-2j} \tag{59}$$

where $\mu=\max(1+\nu-4s,\ 4p+4r-2j+1)$. Minimizing this estimate over M we obtain

$$M_{opt} = C_0\alpha^{-1/\bar{\mu}} \tag{60}$$

where $\bar{\mu}=\max(\nu/2-2s+j,\ 2p+2r)$. We note that $\bar{\mu}=2p+2r$ if

$$j \le 2p + 2r + 2s - \nu/2 . \tag{61}$$

But we know $j\le 2p+2r+1/2$, so if $4s\ge\nu$, then (61) is satisfied, and we have for all $j\le J$ that

$$M_{opt} = C_0\alpha^{-1/(2p+2r)} .$$

Therefore, for $p\ge m/2-r+1/4$ we obtain (57) and for $p<m/2-r+1/4$ the error decreases at least as fast as α^2.

Proof - Part b. Exponentially decaying $|\hat{k}|\ge D\exp(-a\omega)$ for some $a>0$, and all ω. We have assumed that $\hat{k}$ has no real zeros. We again split the error estimate (39) into integrals over $(0,M)$ and (M,∞).

$$\int_0^M |\hat{h}_\alpha|^2 \le \int_0^M \frac{\alpha^2\omega^{4p}e^{4a\omega}|\hat{f}|^2}{D^2+\alpha^2\omega^{4p}e^{4a\omega}} \le \alpha^2 C_1 e^{4aM} \tag{62}$$

Moreover, we obtain (44) again.

Combining (44) and (62) and then minimizing over M, we obtain the transcendental equation for the optimal M

$$4aC_1\alpha^2 e^{4aM} = C_2 M^{-2m-2} .$$

Taking logarithms, we find that the solution

$$M^* \sim -\ln(b\alpha^2)/4a - (\ln((-\ln b\alpha^2)/4a))(m+1)/2a \tag{63}$$

where $b=4aC_1/C_2$. Therefore, a majorant estimate is of the form

$$||h_\alpha||^2 \le C\ (-\ln(b\alpha^2))^{-(2m+1)} . \tag{64}$$

Comments. Part (a) of Theorem 9 states that we can obtain for a larger class of operators the same majorant of the rate of convergence that was obtained in Theorem 5 as long as the growth rate ν of the number of zeros in the interval $(0,M)$ is not greater than 4s. The exponent s in defini-

tion 1 is a measure of the rate of decrease of $\hat{K}$ in a neighborhood of any zero. Part (b) states that for an exponentially decaying operator K the rate of convergence depends primarily on the smoothness of the desired solution and is inversely proportional to $-\ell n\alpha$.

<u>Theorem 10</u>. Consider the norms Ω_p, $p\geq 1$ and equation (1). Let the desired solution f_0 have $m\geq 1$ derivatives with each $f^{(j)} \in L_1(-\infty,\infty)$, $0\leq j\leq m$, and its Fourier transform $\hat{f}$ satisfy $|\omega^{j+1}\hat{f}|\leq R_{j+1}$ for all ω, and $D_2\omega^{-m-1}\geq|\hat{f}|\geq D_1\omega^{-m-1}$ for large ω.

Let K be of type 1 with $0\leq s<1/4$ and $\nu=0$. ($\nu=0$ corresponds to a finite number of zeros.) Moreover, assume $|\hat{K}(\omega)|\leq \bar{D}\omega^{-r}$ as $\omega\uparrow\infty$. Then for sufficiently small α, we obtain the following lower bound:

$$||h_\alpha||^2 \geq Q\alpha^a \quad \text{with } a = (2m+1)/(2p+2r) \tag{65}$$

<u>Proof of Theorem 10</u>. As $\alpha\downarrow 0$, $M(\alpha)$ in (60) becomes arbitrarily large. Therefore, for sufficiently small α, we have

$$||h_\alpha||^2 \geq \int_M^\infty (\alpha^2\omega^{4p+4r}|\hat{f}|^2)/4(\bar{D}+\alpha^2\omega^{4p+4r})$$

Since $M=C_0\alpha^{-1/(2p+2r)}$, we have for $\omega>M$

$$\alpha^2\omega^{4p+4r} > C_0.$$

Therefore, for some Q

$$||h_\alpha||^2 \geq Q\int_M^\infty|\hat{f}|^2 = \bar{Q}M^{-2m-1} = \bar{Q}\alpha^a$$

with $a=(2m+1)/(2p+2r)$. Q.E.D.

<u>Comments</u>. Note that for $p<m/2 - r + 1/4$, the exponent in (65) is greater than 2. So we obtain an order exact estimate for the rate of convergence only for $p\geq m/2 - r + 1/4$, $0\leq s<1/4$ and $\nu=0$.

Next we consider the condition of the approximating problems generated. We again use the dynamic condition, Makhoul [11].

Theorem 11. Consider the norms Ω_p, $p \geq 1$ and equation (1). Let $\hat{K}$ be of type 1 or type 2. Assume moreover that $|\hat{K}|$ is a monotone decreasing function of ω such that $D\omega^{-r} < |\hat{K}(\omega)| < \bar{D}\omega^{-r}$ outside an interval of 0 for type 1, and $C\exp(-a\omega) < |\hat{K}(\omega)| < \bar{C}\exp(-a\omega)$ for all ω for type 2. Then the dynamic condition of the members of the approximating families generated is of order

$$\bar{Q}\alpha^{-r/(p+r)} \tag{66}$$

for type 1 operators and is of order

$$\bar{Q}\alpha^{-1}((-\ln b\alpha)/2a)^{-2p} \tag{67}$$

for type 2 operators where $b = p/ac_i$.

Proof: We consider the operator in the Euler equation (8),

$$\phi \equiv K^*K + \alpha B$$

Part a. type 1 operators

We have that outside an interval of $\omega=0$, $(0,\delta)$,

$$D\omega^{-2r} + \alpha\omega^{2p} \leq |\hat{\phi}(\omega)| \leq \bar{D}\omega^{-2r} + \alpha\omega^{2p} .$$

The minimum of $d\omega^{-2r} + \alpha\omega^{2p}$ occurs when

$$\omega = (rd/2p\alpha)^{1/(2p+2r)} \tag{68}$$

and the corresponding minimum value is

$$Q(d^p\alpha^r)^{1/(p+r)} \tag{69}$$

For small α, ω in (68) is not in $(0,\delta)$. Therefore, the minimum value of $|\hat{\phi}(\omega)|$ lies between the 2 values of (69) obtained for $d = D$ or $\bar{D}$. As we argued in section 3, $|\hat{\phi}|$ has no maximum; however in practice the maximum is limited by the sample size. Therefore, we obtain (66).

Part b. type 2 operators

Using a similar argument for case (b) we obtain the equation

$$\alpha p\omega^{2p-1} = ac\exp(-2a\omega)$$

that we must solve. The solution is approximately

$$\omega^* = (-\ell n b\alpha)/2a - (\ell n((-\ell n b\alpha)/2a))(2p-1)/2a$$

where b=p/ac and the minimum value is

$$|\hat{\phi}(\omega^*)| = Q\alpha((-\ell n b\alpha)/2a)^{2p}$$

Q.E.D.

Comments. We see in Theorem 11 that for operators that decay like ω^{-r}, r>0, increasing the order of Ω has a significant effect upon the condition of the approximating problem generated by the regularization. However, if the decay of K is exponential, then this effect is not great. As indicated in section 2 for operators that decay exponentially, to achieve a condition similar to (66) we must use a norm like Ω_∞^c in (12) or $\overline{\Omega_\infty^c}$ in (23).

Theorem 12. Consider the norms Ω_∞^c and $\overline{\Omega_\infty^c}$ introduced in section 2 equations (12) and (23). Let $\hat{K}$ be of type 1 or type 2, satisfying the hypotheses of Theorem 11. Then the dynamic condition of the members of the approximating families generated is for K of type 1, of the order

$$Q((-\ell n b\alpha)/c)^q \tag{70}$$

where q=2r corresponds to Ω_∞^c, and q=r to $\overline{\Omega_\infty^c}$.

For type 2 operators we obtain for Ω_∞^c, the order

$$Q\alpha^{-d} \quad \text{with } d = 2a/(2a+c) \tag{71}$$

and for $\overline{\Omega_\infty^c}$ the order

$$Q((-\ell n b\alpha)/c)^{1/2}\ . \tag{72}$$

<u>Proof</u> <u>Part a. type 1 operators</u>.

As in the proof of Theorem 11, we compute the minimum of

$$|\hat{\phi}_1| = d\omega^{-2r} + \alpha\cosh c\omega \qquad (73)$$

for Ω_∞^c and of

$$|\hat{\phi}_2| = d\omega^{-2r} + \alpha\exp(c\omega^2) \qquad (74)$$

for $\overline{\Omega_\infty^c}$. Differentiating (73) we obtain

$$\alpha c\omega^{2r+1} = 2rd \ (\sinh c\omega)^{-1}$$

But this equation has the same form as that obtained for case (b) in Theorem 11. Therefore, its approximate solution is given by (63) with some renaming of constants and replacing α^2 by α. Therefore,

$$|\hat{\phi}_1(\omega)| \geq (c/(-\ell n b\alpha))^{2r} \qquad (75)$$

For (74) we obtain

$$\alpha c\omega^{2r+2} = rd\exp(-c\omega^2) \qquad (76)$$

The solution of (76) is approximately

$$c\omega^2 = -\ell n(b\alpha) - (r+1)\ \ell n\ ((-\ell n(b\alpha))/c)$$

where $b=c/rd$. Therefore,

$$|\hat{\phi}_2(\omega)| \geq (c/(-\ell n b\alpha))^r$$

<u>Part b. type 2 operators</u>.

$$|\hat{\phi}_1| = d\exp(-2a\omega) + \alpha\exp(c\omega) \qquad (77)$$

for Ω_∞^c; and for $\overline{\Omega_\infty^c}$,

$$|\hat{\phi}_2| = d\exp(-2a\omega) + \alpha\exp(c\omega^2) \qquad (78)$$

Differentiating (77) and solving for ω we obtain

$$\omega \sim -\ell n(b\alpha)/(2a+c)$$

where $b=c/2ac_1$. Therefore,

$$|\hat{\phi}_1| > Q\alpha^d \quad \text{with } d = 2a/(2a+c).$$

Differentiating (78) and solving for ω we obtain

$$c\omega^2 \sim -\ell n(b\alpha) - \ell n((-\ell nb\alpha)/c)^{1/2}$$

Therefore,

$$|\hat{\phi}_2| \geq (c/(-\ell nb\alpha))^{1/2}(1/b)$$

Combining these estimates we can obtain overall estimates on the error, $||f(\alpha,\varepsilon) - f_0||^2$.

We conclude this section with the following theorem which states that a regularizing family with improved convergence and condition can be used instead of equation (8) if K is symmetric and positive definite.

Theorem 13. If the operator K in (1) is symmetric and positive definite, then for Ω_p, $p\geq 1$ the solutions of the problems $0\leq\alpha\leq 1$

$$(K + \alpha B)f = g \tag{79}$$

with the associated natural boundary conditions form a regularizing family for $Kf=g$ with respect to Ω_p.

We note that the decay rate for K is the square root of that for K*K.

Proof of Theorem 13. Define operators $K_1=\sum\sigma_n^{1/2}u_n u_n^T$ and $K_2= \sum u_n u_n^T/\sigma_n^{1/2}$. Then (79) is the Euler equation for the problem

$$\text{Minimize } ||K_1 f - K_2 g||^2 + \alpha\Omega(f) \ . \tag{80}$$

Equivalently,

$$\text{Minimize } ||Kf - g||^2_{K_3} + \alpha\Omega(f) \tag{81}$$

where $K_3 \equiv \sum u_n u_n^T/\sigma_n$.

We first must show that each of the families (80) and (81) is well-defined. First note that the $\{u_n\}$ are complete since K is invertible.

Moreover, we know that Kf=g has a solution only if

$$\sum (g^T u_n)^2/\sigma_n^2 < \infty .$$

Therefore, $K_1 f$, $K_2 g$ and $K_3 g$ are all well-defined.

We know that f_α minimizes (80) if and only if it satisfies the associated Euler equation. But, due to the symmetry this equation is just (79). But, for example from Tikhonov [13], we know that the solution of (79) converges at least uniformly to the solution of

$$K_1 f = K_2 g \tag{82}$$

as $\alpha \downarrow 0$. But for the given g any solution of (82) is a solution of (1).

Q.E.D.

<u>Comments</u>. Therefore for symmetric, positive definite problems the condition of our approximating problems, if we use (79), is of the order α^b with $b=-r/(2p+r)$, as is the error due to the noise in the data.

5. Summary

In the preceding sections we have considered the question, how does our choice of Ω in (5) affect the condition and the rate of convergence of the approximating problems generated. For convolution equations, the results obtained clearly illustrate the relationship of the condition and the rate of convergence to the choice of norm Ω, the character of the compactness of the operator K, and the smoothness of the desired solution. The condition of the approximating problems generated is strongly dependent upon the order of Ω, and improves as we increase this order. For a given Ω, the condition deteriorates as we increase the decay rate of the singular values of K. The approximations are well-conditioned, if we choose an Ω whose growth rate is at least as fast as the reciprocal of the decay rate of our operator. The rate of convergence depends not only on the compactness of K and the order of Ω but also upon the smoothness of the desired solution. For a given operator K, the smoother the desired solution the better the rate of convergence. This rate deteriorates as either the order of Ω is increased or the decay rate of the operator is increased. With respect to the order of Ω, this deterioration is limited by the smoothness of the desired solution.

The theorems obtained give heuristics for determining the appropriateness of a proposed regularization for a convolution equation. In practice we might not know the smoothness of our solution and would choose a lower order Ω because it is easier to work with. Moreover, we would probably be working on a finite interval, for example $[0,1]$ not $(-\infty,\infty)$.

In an implementation, we have at least 3 ways of solving the minimization problems in (5):

(a) Direct discretization of the functionals in (5) or of the Euler equation in (8).

(b) Solving the Euler equation using Fourier transforms.

(c) Inverting B in (8) with the natural boundary conditions and solving the resulting integral equation of the second kind.

All 3 approaches have been used in practice, see Glasko, Kulik and Tikhonov [13] for approach (a), Anderssen and Bloomfield [14] for approach (b) and Cullum [15] for approach (c). Approach (a) is limited to lower order Ω whereas approach (b) could be used with general regularizers as is done in Aref'eva [6]. In both approaches (a) and (b), if we work with the Euler equation we have the question of satisfying the natural boundary conditions associated with the Euler equation. The statement that (8) is equivalent to (5) includes the boundary conditions. With approach (c) we note that the solution obtained automatically satisfies the natural boundary conditions because we must have

$$\alpha f = B^{-1}(K^*g - K^*Kf). \tag{82}$$

We also note, however, that if we use approach (c), then the resulting operator in (82) is only perturbed by αI from the rapidly decaying operator $B^{-1}K^*K$. Thus, this approach does not seem desirable. However, we can argue that equation (82) is not as bad as it seems. In contrast to what is often done in practice--namely, smoothing the given data and then solving $Kf = g_{smooth}$--in approach (c) we simultaneously smooth the data $B^{-1}K^*g$ and alter the equation. Smoothing the data in this way removes the high

frequency components of the noise in a way consistent with the original equation. To see this consider the following. For B^{-1} generated by (6) the eigenvectors have the oscillation property. That is, if we order the eigenvalues of B^{-1}, μ_n such that $\mu_n \downarrow 0$ as $n \uparrow \infty$, then the number of zero crossings of the eigenvectors $w_n = \sin n\pi t$ $n=1,2...$ (for $n=0$, $w_0=1$) increases as $n \uparrow \infty$. Since the error in the mollified data satisfies

$$B^{-1}K^*\varepsilon = \sum_n (w_n^T K^*\varepsilon)\mu_n w_n ,$$

the high frequency components of $K^*\varepsilon$ (and therefore of ε) are mollified by μ_n.

We could obtain a symmetrized version of (82)

$$\left((B_1 K^* K B_1) + \alpha I\right) h = B_1 K^* g \tag{83}$$

if we could compute $B_1 = B^{-1/2}$. Then h will be derivatives of f, so the solution of (83) may not be as well behaved as that of (82). Once we have (83) we can relate it directly to the results achieved with B=identity, see Hilgers [16]. We note that if instead of using B with the natural boundary conditions, we use another operator with different boundary conditions, see for example Hilgers [16], then the approximations we generate will be good only if the desired solution satisfies these conditions. A comparison of the 3 approaches (a) - (c) is needed.

The preceding discussion demonstrates the importance of one's having some understanding of the given operator K. This can be used to estimate the appropriateness of any proposed regularization, and to give indication of potential difficulties.

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~~We~~ consider ill-posed problems of the form

$$g(t) = \int_0^1 K(t,s)f(s)ds \qquad 0 \le t \le 1 \qquad (1)$$

where g is given and f ~~we~~ must be computed ~~f~~. The Tikhonov regularization procedure replaces (1) by a one-parameter family of minimization prob-

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20. Abstract

(Kf-g) absolute value squared

lems -- Minimize ($||\cancel{Kf - g}||^2$ + $\alpha\Omega(f)$) -- where Ω is a smoothing norm chosen by the user. It is ~~We~~ demonstrated by example that the choice of Ω (Omega) is not simply a matter of convenience. ~~We then show how~~ this choice is shown to affect~~s~~ the convergence rate, and the condition of the problems generated by the regularization. An appropriate choice for Ω (Omega) depends upon the character of the compactness of K and upon the smoothness of the desired solution.